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Computational framework for analyzing fractional biochemical reaction model

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Abstract

The approximate numerical approach for the system of coupled nonlinear ordinary differential equations (ODEs) of a biochemical reaction model is very important for biochemists and scientist working in the field of biochemistry and related issues. Within this article, two computational algorithms for numerically solving a biochemical reaction model with time-fractional derivatives are examined and compared. The first technique depends on the collocation method along with the shifted Jacobi operational matrix for fractional derivative defined in the Caputo sense, and using this technique, we created a system of algebraic equations from the given fractional model. Another approach is centered on the basic theorem of fractional calculus and the characteristics of Newton's polynomial interpolation (NPI). We use these two methods to compute solution for the fractional biochemical reaction model. The model's computational outcomes are compared by using the recommended techniques in this work. Graphical and tabular forms are used to confirm the reliability and effectiveness of both techniques and an excellent match is discovered.

Keywords: Biochemical reaction model, collocation technique, Newton polynomial interpolation, Jacobi operational matrix.

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1. Introduction

Numerous studies and scientists have concentrated on the subject of fractional differential equations over the last few decades. Consequently, a wide range of issues can be simulated and modeled by using fractional differential equations. As an example, in the fields of electrical, electronic, mechanical, biological, and other practical applications. See the work [7, 28] for additional information. Unluckily, it is challenging to attain an accurate solution for these models. The mathematical and estimate techniques have thus captured the attention of a lot of researchers. We have numerous such techniques, including He's variational iteration technique [15, 32], homotopy analysis [25, 33, 34], Fourier spectral techniques [6], Adomian's decomposition technique [38], [43], collocation techniques [8, 19, 20, 44], finite difference

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schemes [47], and spectral techniques [17], [18]. Numerous additional techniques have been used with numerous applied models; for instance, see [2, 26, 48, 49]. Many scholars have shifted their attention towards the topic of fractional calculus in recent years [16, 23, 24, 37, 45, 46].

In biochemical reactions, the outer layer of the enzyme cell automatically has a fractional order electrical conductance [9]. A fractional-order biochemical reaction model has therefore been utilized in this article. This paper uses Caputo version of fractional derivatives because it expertly handles problems with initial values. The usefulness of the collection technique and the Newton polynomial interpolation method to obtain an estimated resolution to well-known Michelson-Menten biochemical reaction model is examined in this article. A straightforward model of the enzymatic process was developed by Michaelis and Menten [27] in 1913, and the basic enzymatic reaction structures have been given by mechanism [35]

$$\Lambda_3 + \Lambda_4 \underset{r_{-1}}{\overset{r_1}{\rightleftharpoons}} \Lambda_2 \xrightarrow{r_2} \Lambda_3 + \Lambda_1,$$

where the letters Λ_3, Λ_4, Λ_2, and Λ_1 stand for the respective enzyme, substrate, intermediate complex, and product. For each reaction, the variables r_1, r_{-1}, and r_2, respectively, show the positive rate constants. The mass action principle states that, concentrations of the reactants directly affect reaction rates then it is possible to calculate the above scheme's time evolution from the four nonlinear ODE system's solution [36],

$$\frac{d\Lambda_4}{dt} = -r_1\Lambda_3\Lambda_4 + r_{-1}\Lambda_2, \qquad \frac{d\Lambda_3}{dt} = -r_1\Lambda_3\Lambda_4 + (r_{-1}+r_2)\Lambda_2,$$
$$\frac{d\Lambda_2}{dt} = r_1\Lambda_3\Lambda_4 - (r_{-1}+r_2)\Lambda_2, \quad \frac{d\Lambda_1}{dt} = r_2\Lambda_2,$$

depending on the initial circumstances: $\Lambda_4(0) = \Lambda_0^4$, $\Lambda_3(0) = \Lambda_0^3$, $\Lambda_2(0) = 0$, $\Lambda_1(0) = 0$. There are only two equations that can be used in place of the differential equations mentioned above for the substrate Λ_4 and the intermediate enzyme-substrate complex Λ_2 [12]. With derivatives of fractional order ϵ, the new set of DE is given by

$$\frac{d^\epsilon\lambda_1}{dt^\epsilon} = -\lambda_1 + (\zeta-\eta)\lambda_2 + \lambda_1\lambda_2, \ \ 0 < \epsilon \leqslant 1, \qquad \frac{d^\epsilon\lambda_2}{dt^\epsilon} = \frac{1}{\gamma}(\lambda_1 - \zeta\lambda_2 - \lambda_1\lambda_2), \ \ 0 < \epsilon \leqslant 1, \tag{1.1}$$

depending on the initial situations: $\lambda_1(0) = 1, \lambda_2(0) = 0$, where λ_1 and λ_2 represent the substrate and enzyme-substrate intermediate complex concentrations, respectively, in dimensionless form. To get more general results we change standard order differential equations into fractional differential equations.

2. Preliminaries

2.1. An introduction to fractional calculus

The definitions used for the concept and the characteristics that are going to be utilized during this study are presented here [21, 29].

Definition 2.1. For $\epsilon > 0$ and $\lambda(t) \in H_1(c,d)$, where $H_1(c,d)$ is the space of all integrable functions on (c, d), Riemann-Liouville fractional integral of order ϵ, indicated by I_0^ϵ, is provided by

$$I_0^\epsilon\lambda(t) = \frac{1}{\Gamma(\epsilon)}\int_0^t (t-\phi)^{\epsilon-1}\lambda(\phi)d\phi.$$

Definition 2.2. The Caputo fractional derivative of order ϵ, for $\epsilon > 0$, indicated by D^ϵ, is described by

$$D^\epsilon\lambda(t) = \frac{1}{\Gamma(m-\epsilon)}\int_0^t (t-\phi)^{m-\epsilon-1}D^m\lambda(\phi)d\phi \quad (m-1 < \epsilon < m; m \in \mathbb{N} = \{1,2,3,\ldots\}).$$

If derivatives signs $\frac{d^\epsilon}{dt^\epsilon}$ are replaced in (1.1) by D^ϵ and $0 < \epsilon \leqslant 1$, we attain the fractional biochemical reaction model in sense of Caputo derivative as

$$ {}_0D_t^\epsilon \lambda_1(t) = -\lambda_1 + (\zeta - \eta)\lambda_2 + \lambda_1\lambda_2, \tag{2.1}$$

$$ {}_0D_t^\epsilon \lambda_2(t) = \frac{1}{\gamma}(\lambda_1 - \zeta\lambda_2 - \lambda_1\lambda_2). \tag{2.2}$$

2.2. Function approximation

A function $\rho \in L_f^2[0,1]$, with $|\rho''(y)| \leqslant A$, can be extended as

$$ \rho(y) = \lim_{k\to\infty} \sum_{r=0}^{k} o_r u_r^{(p,q)}(y), \tag{2.3}$$

$\rho(y) =< o_r, u_r^{(p,q)}(y) >$ and sign $< .,. >$ represents standard inner product. Regarding estimation of finite dimension this is the composition of equation (2.3),

$$ \rho \cong \sum_{r=0}^{m} o_r u_r^{(p,q)}(y) = O^T U_m(y).$$

Matrices $U_m(y)$ and O are of order $(m+1)\times 1$, given as

$$ O = [o_0, o_1, \ldots, o_m]^T \quad \text{and} \quad U_m(y) = [u_0^{(p,q)}, u_1^{(p,q)}, \ldots, u_m^{(p,q)}]^T.$$

2.3. Jacobi polynomials

This article uses Jacobi polynomials as a foundation for estimating unknown functions. The definition of the shifted Jacobi polynomial is [1, 5, 11]:

$$ u_r^{(g,h)}(y) = \sum_{e=0}^{r} (-1)^{r-e} \frac{\Gamma(r+h+1)\Gamma(r+e+g+h+1)}{\Gamma(e+h+1)\Gamma(r+g+h+1)(r-e)!e!} y^e,$$

where the parameters of the Jacobi polynomial, described in Doha et al. [11], are p and q. Orthogonal property of Jacobi polynomials are

$$ \int_0^1 u_i^{(g,h)}(y) u_s^{(g,h)}(y) \omega^{(g,h)}(y) dy = \psi_i^{g,h} \delta_{is},$$

δ_{is} and $\omega^{(g,h)}(y)$ denote Kronecker delta function and weight function, respectively, displayed as

$$ \omega^{(g,h)}(y) = (1-y)^g y^h \quad \text{and} \quad \psi_i^{g,h} = \frac{\Gamma(i+g+1)\Gamma(i+h+1)}{(2i+g+h+1)k!\Gamma(i+g+h+1)}.$$

2.4. Fractional derivative Jacobi operational matrix

Theorem 2.3. *Assuming that* $U_k(y) = [u_0^{(p,q)}, u_1^{(p,q)}, \ldots, u_k^{(p,q)}]^T$ *is the shifted Jacobi vector and* $\epsilon > 0$, *then*

$$ D^\epsilon u_r^{(g,h)}(y) = D^{(\epsilon)} U_k(y).$$

Here $D^{(\epsilon)} = (M(r,j))$ *denotes operational matrix of order* $(k+1)\times(k+1)$, *and* ϵ *represent order of fractional derivative, which entries are provided as*

$$ M(r,j,g,h) = \sum_{a=[\epsilon]}^{r} (-1)^{r-a} \frac{\Gamma(r+g+1)\Gamma(r+a+g+h+1)}{(r-a)!\Gamma(a+h+1)\Gamma(r+g+h+1)\Gamma(a-\epsilon+1)}$$
$$ \times \sum_{s=0}^{j} (-1)^{j-s} \frac{\Gamma(g+1)\Gamma(j+s+g+h+1)\Gamma(a+s-\epsilon+h+1)(2j+g+h+1)j!}{(j-s)!(s)!\Gamma(j+g+1)\Gamma(s+h+1)\Gamma(a+s-\epsilon+g+h+2)}.$$

Proof. Research papers [1, 5, 11] are available to view as evidence. □

3. An overview of the methodology

In this section, we will look at the procedure that makes use of collocation technique and operational matrix to produce fractional DE solution [39–41]. First of all, we adopt following estimation:

$$\lambda(t) = \sum_{r=0}^{k} o_r u_r^{(p,q)}(t) = O^T U_k(t). \tag{3.1}$$

Taking order one derivative of (3.1), we obtain

$$D'\lambda(t) = O^T D' U_k(t) \cong O^T D^{(1)} U_k(t), \tag{3.2}$$

$D^{(1)}$ is operational differentiation matrix of order 1. Now, taking order ϵ derivative of (3.1),

$$D^{\epsilon}\lambda(t) = O^T D^{\epsilon} U_k(t) \cong O^T D^{(\epsilon)} U_k(t), \tag{3.3}$$

$D^{(\epsilon)}$ is operational differentiation matrix of order ϵ. From (3.1) and (3.2), we can write

$$\lambda(0) = O^T U_k(0), \qquad \lambda'(0) = O^T D^{(1)} U_k(0). \tag{3.4}$$

3.1. Numerical simulation of the fractional order biochemical reaction mode

In equations (2.1) and (2.2), using (3.1) and (3.3) we attain following equations:

$$O_1^T D^{(\epsilon)} U_k(t) + O_1^T U_k(t) - (\zeta - \eta) O_2^T U_k(t) - O_1^T U_k(t) O_2^T U_k(t) = 0, \tag{3.5}$$

$$O_2^T D^{(\epsilon)} U_k(t) - \frac{1}{\gamma}\left(O_1^T U_k(t) - \zeta O_2^T U_k(t) - O_1^T U_k(t) O_2^T U_k(t)\right) = 0. \tag{3.6}$$

The residuals for Equations (3.5) and (3.6) are given as:

$$R_{1k}(t) = O_1^T D^{(\epsilon)} U_k(t) + O_1^T U_k(t) - (\zeta - \eta) O_2^T U_k(t) - O_1^T U_k(t) O_2^T U_k(t), \tag{3.7}$$

$$R_{2k}(t) = O_2^T D^{(\epsilon)} U_k(t) - \frac{1}{\gamma}\left(O_1^T U_k(t) - \zeta O_2^T U_k(t) - O_1^T U_k(t) O_2^T U_k(t)\right). \tag{3.8}$$

Now, when Equations (3.7) and (3.8) are collocated at k points presented as $t_r = \frac{r}{k}$, $r = 0, 1, 2, \ldots, k-1$, we get

$$R_{1k}(t_r) = O_1^T D^{(\epsilon)} U_k(t_r) + O_1^T U_k(t_r) - (\zeta - \eta) O_2^T U_k(t_r) - O_1^T U_k(t_r) O_2^T U_k(t_r), \tag{3.9}$$

$$R_{2k}(t_r) = O_2^T D^{(\epsilon)} U_k(t_r) - \frac{1}{\gamma}\left(O_1^T U_k(t_r) - \zeta O_2^T U_k(t_r) - O_1^T U_k(t_r) O_2^T U_k(t_r)\right). \tag{3.10}$$

Using equation (3.4), the initial conditions become as follows:

$$O_1^T U_k(0) - \lambda_1(0) = 0, \qquad O_2^T U_k(0) - \lambda_2(0) = 0, \tag{3.11}$$

A non-linear set of $2(k+1)$ equations is produced by equations (3.9) and (3.10) and the initial conditions (3.11). We obtain O_1^T and O_2^T values from the system's solution. We can easily find an approximated solution of the fractional differential equations (2.1)-(2.2) after getting the unknown values.

4. Error analysis

Theorem 4.1. *Let* $\lambda : [0,1] \longrightarrow \mathbb{R}$ *be a function,* $\lambda \in C^{(k+1)}[0,1]$, *and* $\lambda_k(y)$*be the* k^{th} *approximate discovered using Jacobi polynomials. Then*

$$E^f_{\lambda,k} = \|\lambda - \lambda_k\|_{L^2_f[0,1]},$$

as $k \longrightarrow \infty$ *and error vector* $E^f_{\lambda,k} \longrightarrow 0$.

Proof. Refer to the books of Rivlin [30] and Kreyszig [22], as well as the research study by Behroozifar and Sazmand [4]. □

Theorem 4.2. $E^{\epsilon,f}_{D,k}$ *is the error vector for the* ϵ *order operational matrix differentiation, which takes place using* $(k+1)$ *Jacobi polynomials. Then*

$$E^{\epsilon,f}_{D,k} = D^{(\epsilon)}U_k(t) - D^{\epsilon}U_k(t), \tag{4.1}$$

the error vector of Equation (4.1) *tends towards zero as* $k \longrightarrow \infty$.

Proof. The studies of Ezz-Eladien et al. [14] and Singh and Srivastava [42] are available for viewing it. □

Theorem 4.3. *Consider the functional G, then*

$$\lim_{k\to\infty} \alpha_k(t) = \alpha(t) = \inf_{t\in[0,1]} G(t).$$

Proof. See [13]. □

For equation (2.1), the functional G is given as

$$G(t) = {}_0D^{\epsilon}_t\lambda_1(t) + \lambda_1(t) - (\zeta-\eta)\lambda_2(t) - \lambda_1(t)\lambda_2(t) = 0. \tag{4.2}$$

Using equations (3.1) and (3.3), we obtain

$$\begin{aligned} G^{(E)}(t) = {} & O_1^T D^{(\epsilon)}U_k(t) + E^{\epsilon,f}_{D,k} + O_1^T U_k(t) + E^f_{\lambda,k} - (\zeta-\eta)\big(O_2^T U_k(t) + E^f_{\lambda,k}\big) \\ & - \big(O_1^T U_k(t) + E^f_{\lambda,k}\big)\big(O_2^T U_k(t) + E^f_{\lambda,k}\big), \end{aligned} \tag{4.3}$$

where

$$E^f_{\lambda,k} = O^T U(t) - O^T U_k(t), \qquad E^{\epsilon,f}_{D,k} = D^{(\epsilon)}U_k(t) - D^{\epsilon}U_k(t).$$

Residual for equation (4.3) is

$$\begin{aligned} R^{(E)}_k(t) = {} & O_1^T D^{(\epsilon)}U_k(t) + E^{\epsilon,f}_{D,k} + O_1^T U_k(t) + E^f_{\lambda,k} - (\zeta-\eta)\big(O_2^T U_k(t) + E^f_{\lambda,k}\big) \\ & - \big(O_1^T U_k(t) + E^f_{\lambda,k}\big)\big(O_2^T U_k(t) + E^f_{\lambda,k}\big), \end{aligned}$$

when equation (4.3) is collocated at k points presented by $t_r = \frac{r}{k}$, $r = 0,1,2,\ldots,k-1$, we obtain

$$\begin{aligned} R^{(E)}_k(t_r) = {} & O_1^T D^{(\epsilon)}U_k(t_r) + E^{\epsilon,f}_{D,k} + O_1^T U_k(t_r) + E^f_{\lambda,k} \\ & - (\zeta-\eta)\big(O_2^T U_k(t_r) + E^f_{\lambda,k}\big) - \big(O_1^T U_k(t_r) + E^f_{\lambda,k}\big)\big(O_2^T U_k(t_r) + E^f_{\lambda,k}\big). \end{aligned} \tag{4.4}$$

Equations (4.4) and (3.11) together yield a set of non-linear algebraic equations in the final step. To obtain value of the unknowns we solve the attain system, and after that, we solve Equation (4.2). Let $\alpha^*_k(t)$ represent the achieved solution. Now, utilizing Theorems 4.1 and 4.2 and applying the limit $k \longrightarrow \infty$,

$$\alpha^*_k(t) \longrightarrow \alpha_k(t). \tag{4.5}$$

From (4.5) and Theorem 4.3, $\lim_{k\to\infty} \alpha_k(t) = \alpha(t)$. For the fractional differential equation (2.2), the identical proof can be created.

5. Newton polynomial interpolation

In order to explore the arithmetical solutions of the suggested fractional biochemical reaction model, this part will develop iterative formulas and use them to get numerical solution ([3, 31]). For equations (2.1) and (2.2), the fundamental theorem of fractional calculus yields iterative formulas

$$\lambda_1(t)-\lambda_1(0)=\frac{1}{\Gamma(\epsilon)}\int_0^t(-\lambda_1(\phi)+(\zeta-\eta)\lambda_2(\phi)+\lambda_1(\phi)\lambda_2(\phi))\,(t-\phi)^{\epsilon-1}d\phi, \tag{5.1}$$

$$\lambda_2(t)-\lambda_2(0)=\frac{1}{\Gamma(\epsilon)}\int_0^t\left(\frac{1}{\gamma}(\lambda_1(\phi)-\zeta\lambda_2(\phi)-\lambda_1(\phi)\lambda_2(\phi))\right)(t-\phi)^{\epsilon-1}d\phi. \tag{5.2}$$

These equations (5.1) and (5.2) can be rewritten as

$$\lambda_1\,(t_{n+1})-\lambda_1(0)=\frac{1}{\Gamma(\epsilon)}\sum_{m=2}^{\infty}\int_{t_m}^{t_{m+1}}(-\lambda_1(\phi)+(\zeta-\eta)\lambda_2(\phi)+\lambda_1(\phi)\lambda_2(\phi))\,(t_{m+1}-\phi)^{\epsilon-1}d\phi,$$

$$\lambda_2\,(t_{n+1})-\lambda_2(0)=\frac{1}{\Gamma(\epsilon)}\sum_{m=2}^{\infty}\int_{t_m}^{t_{m+1}}\left(\frac{1}{\gamma}(\lambda_1(\phi)-\zeta\lambda_2(\phi)-\lambda_1(\phi)\lambda_2(\phi))\right)(t_{m+1}-\phi)^{\epsilon-1}d\phi.$$

We use Newton polynomial interpolation to derive the results (same as in [3])

$$\begin{aligned}
\lambda_1(t_{n+1})&=\lambda_1(0)+\frac{1}{\Gamma(\epsilon)}\sum_{m=2}^{n}(-\lambda_1(t_{m-2})+(\zeta-\eta)\lambda_2(t_{m-2})+\lambda_1(t_{m-2})\lambda_2(t_{m-2}))\\
&\times\int_{t_m}^{t_{m+1}}\frac{1}{(t_{n+1}-\phi)^{1-\epsilon}}d\phi+\frac{1}{h\Gamma(\epsilon)}\sum_{m=2}^{n}\big((-\lambda_1(t_{m-1})+(\zeta-\eta)\lambda_2(t_{m-1})+\lambda_1(t_{m-1})\lambda_2(t_{m-1}))\\
&-\big(-\lambda_1(t_{m-2})+(\zeta-\eta)\lambda_2(t_{m-2})+\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\big)\\
&\times\int_{t_m}^{t_{m+1}}\frac{(\phi-t_{m-2})}{(t_{n+1}-\phi)^{1-\epsilon}}d\phi+\frac{1}{2h^2\Gamma(\epsilon)}\sum_{m=2}^{n}\big((-\lambda_1(t_m)(\zeta-\eta)\lambda_2(t_m)+\lambda_1(t_m)\lambda_2(t_m))\\
&-2\,(-\lambda_1(t_{m-1})+(\zeta-\eta)\lambda_2(t_{m-1})+\lambda_1(t_{m-1})\lambda_2(t_{m-1}))+\big(-\lambda_1(t_{m-2})+(\zeta-\eta)\lambda_2(t_{m-2})\\
&+\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\big)\int_{t_m}^{t_{m+1}}\frac{(\phi-t_{m-2})(\phi-t_{m-1})}{(t_{n+1}-\phi)^{1-\epsilon}}d\phi,\\
\lambda_2(t_{n+1})&=\lambda_2(0)+\frac{1}{\Gamma(\epsilon)}\sum_{m=2}^{n}\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-2})-\zeta\lambda_2(t_{m-2})-\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\right)\int_{t_m}^{t_{m+1}}\frac{1}{(t_{n+1}-\phi)^{1-\epsilon}}d\phi\\
&+\frac{1}{h\Gamma(\epsilon)}\sum_{m=2}^{n}\left(\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-1})-\zeta\lambda_2(t_{m-1})-\lambda_1(t_{m-1})\lambda_2(t_{m-1})\big)\right)-\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-2})-\zeta\lambda_2(t_{m-2})\right.\right.\\
&\left.\left.-\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\right)\right)\int_{t_m}^{t_{m+1}}\frac{(\phi-t_{m-2})}{(t_{n+1}-\phi)^{1-\epsilon}}d\phi+\frac{1}{2h^2\Gamma(\epsilon)}\sum_{m=2}^{n}\left(\left(\frac{1}{\epsilon}\big(\lambda_1(t_m)-\zeta\lambda_2(t_m)\right.\right.\\
&\left.\left.-\lambda_1(t_m)\lambda_2(t_m)\big)\right)-2\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-1})-\zeta\lambda_2(t_{m-1})-\lambda_1(t_{m-1})\lambda_2(t_{m-1})\big)\right)\right.\\
&\left.+\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-2})-\zeta\lambda_2(t_{m-2})-\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\right)\right)\int_{t_m}^{t_{m+1}}\frac{(\phi-t_{m-2})(\phi-t_{m-1})}{(t_{n+1}-\phi)^{1-\epsilon}}d\phi.
\end{aligned}$$

This Newton interpolation formula evaluates the integrals directly. The computational solutions to equations (2.1) and (2.2) are then given using the Caputo derivative,

$$\lambda_1(t_{n+1})=\lambda_1(0)+\frac{h^{\epsilon}}{\Gamma(1+\epsilon)}\sum_{m=2}^{n}(-\lambda_1(t_{m-2})+(\zeta-\eta)\lambda_2(t_{m-2})+\lambda_1(t_{m-2})\lambda_2(t_{m-2}))\,\Omega_1+\frac{h^{\epsilon}}{\Gamma(2+\epsilon)}$$

$$\times \sum_{m=2}^{n}\Big((-\lambda_1(t_{m-1})+(\zeta-\eta)\lambda_2(t_{m-1})+\lambda_1(t_{m-1})\lambda_2(t_{m-1}))-\big(-\lambda_1(t_{m-2})+(\zeta-\eta)\lambda_2(t_{m-2})$$
$$+\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\Big)\Omega_2+\frac{h^{\epsilon}}{2\Gamma(3+\epsilon)}\sum_{m=2}^{n}\Big((-\lambda_1(t_m)+(\zeta-\eta)\lambda_2(t_m)+\lambda_1(t_m)\lambda_2(t_m))$$
$$-2\,(-\lambda_1(t_{m-1})+(\zeta-\eta)\lambda_2(t_{m-1})+\lambda_1(t_{m-1})\lambda_2(t_{m-1}))+\big(-\lambda_1(t_{m-2})+(\zeta-\eta)\lambda_2(t_{m-2})$$
$$+\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\Big)\Omega_3,$$

$$\lambda_2(t_{n+1})=\lambda_2(0)+\frac{h^{\epsilon}}{\Gamma(1+\epsilon)}\sum_{m=2}^{n}\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-2})-\zeta\lambda_2(t_{m-2})-\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\right)\Omega_1+\frac{h^{\epsilon}}{\Gamma(2+\epsilon)}$$
$$\times\sum_{m=2}^{n}\left(\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-1})-\zeta\lambda_2(t_{m-1})-\lambda_1(t_{m-1})\lambda_2(t_{m-1})\big)\right)-\Big(\frac{1}{\epsilon}\big(\lambda_1(t_{m-2})-\zeta\lambda_2(t_{m-2})\right.$$
$$\left.-\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\Big)\right)\Omega_2+\frac{h^{\epsilon}}{2\Gamma(3+\epsilon)}\sum_{m=2}^{n}\left(\left(\frac{1}{\epsilon}\big(\lambda_1(t_m)-\zeta\lambda_2(t_m)-\lambda_1(t_m)\lambda_2(t_m)\big)\right)\right.$$
$$-2\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-1})-\zeta\lambda_2(t_{m-1})-\lambda_1(t_{m-1})\lambda_2(t_{m-1})\big)\right)$$
$$\left.+\left(\frac{1}{\epsilon}\big(\lambda_1(t_{m-2})-\zeta\lambda_2(t_{m-2})-\lambda_1(t_{m-2})\lambda_2(t_{m-2})\big)\right)\right)\Omega_3,$$

where

$$\Omega_1=(n-m+1)^{\epsilon}-(n-m)^{\epsilon},$$
$$\Omega_2=(n-m+1)^{\epsilon}(n-m+3+2\epsilon)-(n-m)^{\epsilon}(n-m+3+3\epsilon),$$
$$\Omega_3=(n-m+1)^{\epsilon}\left(2(n-m)^2+(3\epsilon+10)(n-m)+2\epsilon^2+9\epsilon+12\right)$$
$$-(n-m)^{\epsilon}\left(2(n-m)^2+(5\epsilon+10)(n-m)+6\epsilon^2+18\epsilon+12\right).$$

6. Numerical results and discussion

This part of the article specifically examines the effect of fractional order ϵ on the concentration of the substrate and an intermediate enzyme-substrate complex. Distinct values of the fractional order ϵ for the dimensionless reaction parameters $\zeta = 1$, $\eta = 0.375$, and $\gamma = 0.1$ are taken into consideration in the numerical solution of the fractional order biochemical reaction model utilizing the collection technique and NPI method. For multiple values of fractional order, $\epsilon = 0.90,\ 0.80,\ 0.70$, as well as for the classical derivative order, $\epsilon = 1$, the estimated outcomes of $\lambda_1(t)$ and $\lambda_2(t)$ are calculated. The graphical outcomes by collocation technique are shown in Figures 1 and 2. The analysis concludes that fractional order continuously influences the mathematical solutions that were acquired. Additionally, it is visible that as ϵ approaches 1, computational solutions of the fractional biochemical reaction model approach the accurate solutions. With an increasing value of t and decreasing value of ϵ, Figure 1 shows that concentration of substrate, i.e., $\lambda_1(t)$, reduces and then further tends to zero. Figure 2 shows that as t is increased and ϵ is decreased, concentration of the intermediate enzyme-substrate complex, denoted by the symbol $\lambda_2(t)$, rises and reaches its maximum value. The behavior of $\lambda_1(t)$ and $\lambda_2(t)$ concerning time are also shown in Figure 3 and 4 and these figures are obtained by Newton's polynomial interpolation technique ($\epsilon = 1$, $L = 0.1$, $h = 0.0002$, $\zeta = 1$, $\eta = 0.375$, $\gamma = 0.1, n = 500$). Figures 5 and 6 demonstrate the comparison of the computational solutions of fractional biochemical reaction model using two proposed methodology. Additionally, we see in these graphs that the numerical results for the two approaches are very similar and display the same behavior. The outcome is well-aligned with the results of the fractional homotopy analysis transform technique and multistage new iterative technique utilized, respectively, by Damarla et al. [10] and Dubey et al. [12] for the fractional biochemical reaction model.

Table 1: A comparison of the $\lambda_1(t)$ numerical value calculated by Jacobi collocation method (JCM) and Newton polynomial interpolation (NPI) method for $\epsilon = 1$.

t	λ_1(JCM)	λ_1(NPI)
0.00	1	1
0.02	0.982703	0.983288
0.04	0.969802	0.970765
0.06	0.960045	0.961251
0.08	0.952484	0.953722
0.10	0.946413	0.947514

Table 2: A comparison of the $\lambda_2(t)$ numerical value calculated by Jacobi collocation method (JCM) and Newton polynomial interpolation (NPI) method for $\epsilon = 1$.

t	λ_2(JCM)	λ_2(NPI)
0.00	0	0
0.02	0.166948	0.160807
0.04	0.280173	0.269614
0.06	0.354985	0.341654
0.08	0.402998	0.389399
0.10	0.432846	0.421011

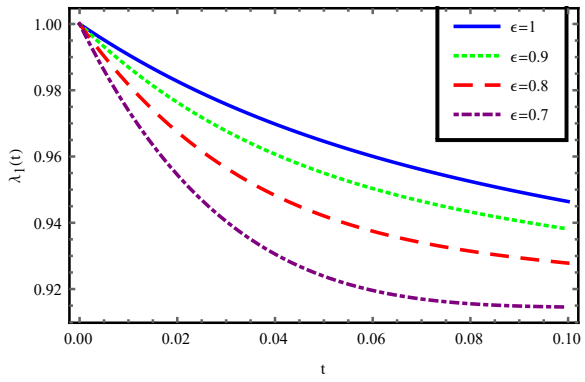

Figure 1: Plot of $\lambda_1(t)$ vs t for various fractional order obtained by collocation technique at $g = 1$ $h = 1$, $k = 8$, $\zeta = 1$, $\eta = 0.375$, $\gamma = 0.1$.

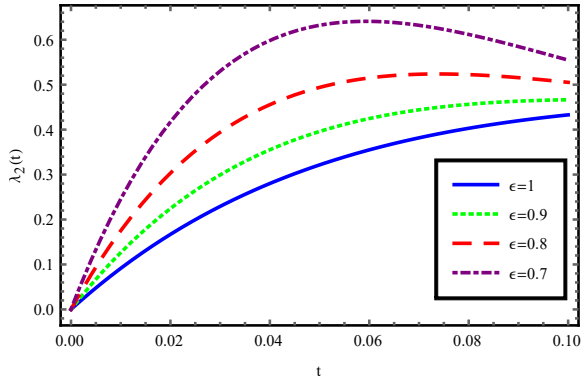

Figure 2: Plot of $\lambda_2(t)$ vs t for various fractional order obtained by collocation technique at $g = 1$ $h = 1$, $k = 8$, $\zeta = 1$, $\eta = 0.375$, $\gamma = 0.1$.

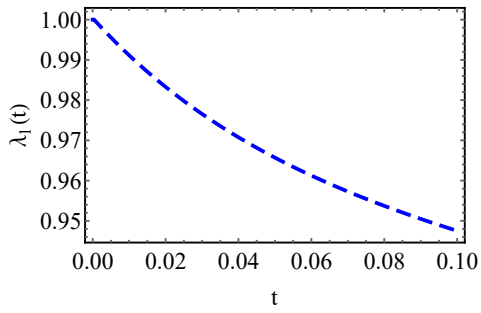

Figure 3: Plot $\lambda_1(t)$ vs t for fractional order $\epsilon = 1$ obtained by NPI technique at $L = 0.1$, $h = 0.0002$, $n = 500$, $\zeta = 1$,$\eta = 0.375$, $\gamma = 0.1$.

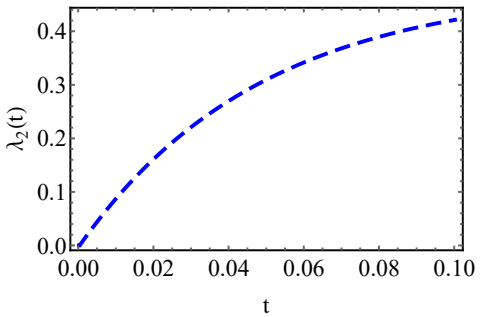

Figure 4: Plot $\lambda_2(t)$ vs t for fractional order $\epsilon = 1$ obtained by NPI technique at $L = 0.1$, $h = 0.0002$, $n = 500$, $\zeta = 1$,$\eta = 0.375$, $\gamma = 0.1$.

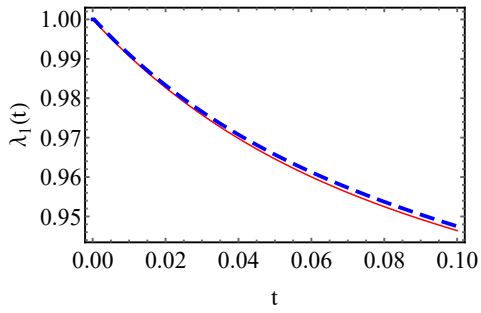

Figure 5: Graph of $\lambda_1(t)$ vs t for $\epsilon = 1$ obtained by collocation technique (line) and NPI technique (dash line).

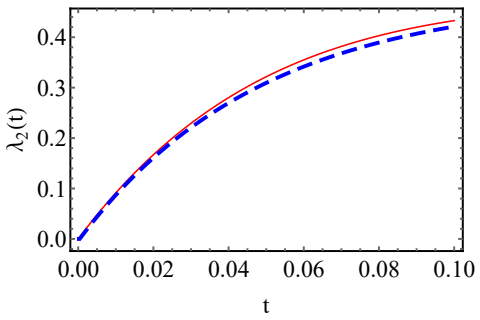

Figure 6: Graph of $\lambda_2(t)$ vs t for $\epsilon = 1$ obtained by collocation technique (line) and NPI technique (dash line).

7. Conlusions

In this article, two computational methodologies are discussed to evaluate the computational solutions of the fractional biochemical reaction model. The first approach depends on the Jacobi polynomials' operational matrix and collocation technique. The basic concept of fractional calculus and Newton's polynomial interpolation are used for constructing the second technique. To find mathematical solutions to the fractional biochemical reaction model, these two techniques are used. The graphs produced by the two recommended approaches were combined to compare the numerical solutions and a good compatibility was discovered. The fractional biochemical reaction model's mathematical solution utilizing collocation method and NPI technique demonstrate how effectively these methods can be applied to explain chemistry-related issues in chemistry science.

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